

## Chairman's Message

### CCP13 NEWS

The CCP13 Newsletter continues to go from strength to strength and this year, by popular demand, has been given a meatier title the 'Fibre Diffraction Review'. Following on from the successful improvement in presentation of the last (1995) issue, this edition, the fifth Newsletter, builds on this success and includes discussion of some of the recent topics taxing fibre diffractionists at the present time. It also includes abstracts from the 1996 CCP13/NCD Workshop at the Daresbury Laboratory which has become a regular feature. Additional copies of the Fibre Diffraction Review have been printed so that it will go not only to people on the CCP13 mailing list, but also to places and people regarded as influential and potentially interested or supportive. In addition, the Fibre Diffraction Review is being incorporated as part of the CCP13 World Wide Web pages (as with the previous Newsletters: details elsewhere). Articles in the current edition of the Fibre Diffraction Review illustrate some of the progress made in developing CCP13 fibre diffraction software in the past year, some ideas about the direction that CCP13 should take in the future, and application of the existing suite to a range of interesting biological and materials science problems.

As detailed in the report by G.Mant, the 1996 Annual Workshop at Daresbury was, once again, a joint meeting, with an international flavour, of CCP13 and the UK Non-Crystalline Diffraction community, reflecting the considerable overlap of interests of the two groups. The meeting was very well attended and emphasises the importance of the topic. The success of the format means that the 1997 meeting will be structured in a related way, although this time, as an experiment, being scheduled over two days rather than three. Remember not only that your poster could win a large cash prize (1st Prize - £100; 2nd Prize - £50), but also that abstracts will be included in this Annual 'Fibre Diffraction Review' (also on the WWW) - your work will be available to a worldwide audience. As usual, there will be bursaries available for students and young scientists to attend the 1997 Workshop. Details of all these are given at the end of the Newsletter.

CCP stands for Collaborative Computational Project. CCP13 is funded in the UK mainly by the Biotechnology and Biological Sciences Research

Council (BBSRC). An additional grant comes from EPSRC to help fund meetings and travel for the 'synthetic polymer' side of CCP13. CCP13 is one of 12 current CCPs run mainly by BBSRC/EPSRC. Our current CCP runs to the end of September, 1998 with BBSRC support. A CCP Steering Committee has been formed to coordinate activities of all the CCPs. The Chairman of the Committee is Prof. Dominic Tildsley (Imperial College) and the Secretary is Dr. Paul Durham (Daresbury). This Steering Committee has met twice so far and is gradually formulating the role it should play in future CCP activities.

The current BBSRC grant to CCP13 allows the continued employment of Richard Denny as the CCP13 RA and it provides funds towards Workshops, Newsletter Production and International Interactions. The funding by BBSRC and EPSRC also allows CCP13 to carry out 'good works'. At the last CCP13 Workshop it was agreed that these would be to fund a small number of 'CCP13 Travelling Fellowships' and a 'CCP13 Visiting Scientist Fellowship Program'. This year we awarded our 'CCP13 Visiting Scientist Fellowship' to Prof. Rick Millane, from the Whistler Center for Carbohydrate Research at Purdue University. Prof. Millane not only participated in the 1996 CCP13/NCD Workshop, but also visited various laboratories around the UK and gave lectures. His report is included elsewhere in this edition.

The two CCP13 Travelling Fellowships were awarded to Dr. Jeff Harford (Imperial College) and Dr. Patrick Fairclough (UMIST). Reports on their visits are also reported here. Application details for Travelling fellowships to be awarded during 1997 are given later in this issue.

### Your Contribution

Interested groups or individuals are invited to contact any of the officers of CCP13 to obtain information about CCP13 Workshops, software developments, software standards and so on. Offers of home-written software that could be incorporated into the new CCP13 suite of programs would be much appreciated and will, of course, permanently carry the authors' attribution. Make sure that you are on the CCP13 mailing list and you will be kept informed.



## Editorial Policy

Articles for inclusion in the Fibre Diffraction Review are welcome by the Editor at any time, but preferably items for the December 1997 issue should arrive before the end of November 1997. It is hoped that the Fibre Diffraction Review will become an Annual 'essential' for Fibre Diffractionists. This is the place to advertise your fibre diffraction or NCD meetings, to report on new software or 'hot' results obtained using the CCP13 or other fibre pattern processing suites and to provide reports of meetings of interest, preferably together with one or two photographs. All technical articles will be scrutinised both for scientific content and presentational style by the Editor (or his nominee) together with at least one other member of the CCP13 Steering Panel. In this way we hope to maintain high standards. Remember that the Newsletter not only goes to other Fibre Diffractionists, but also to various members of the Research Council Secretariats and to other funding agencies.

## International Cooperation

Although these CCPs are UK funded projects, there is a very strong interest in making them international through cooperation with interested scientists in other countries. A natural link for CCP13, for example, exists with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association and possibly with some

American synchrotron users (CHESS). Others exist with the ESRF at Grenoble and with the Photon Factory in Japan.

## Retirements and New Elections

At the 1996 Annual Meeting, John Squire was re-elected as CCP13 Chairman, Geoff Mant was re-elected as Secretary and Manolis Pantos was re-elected as a Committee member. Unfortunately, Dr. Rob Rule tendered his resignation from the Committee in November 1996. Rob's job has moved and he now has new commitments that make it difficult for him to continue. However, he has made a major contribution to our activities for a number of years and I am happy to express, on behalf of CCP13, our considerable appreciation of his role in helping to get CCP13 off the ground and into the healthy position that it now enjoys. The CCP13 Committee are now seeking a replacement for him. The term of office of Tony Ryan finishes at the May meeting this year; other existing Committee members all continue at least until 1998. There are therefore two positions to be filled at the CCP13 Annual General Meeting in May. Tony Ryan is prepared to stand again for election to the Committee. Other nominations for election to the Committee can be sent to the CCP13 Secretary, Dr. Geoff Mant, before the May 1997 meeting.

John Squire

**IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS. THIS CCP IS FOR YOU. PLEASE HELP TO MAKE IT WORK!**

## 1996 IUCr, Seattle

The main focus of this CCP13 sponsored visit over 10 days (August 12-22, 1996) to the USA was the attendance and presentation of an invited paper at the XVII IUCr (International Union of Crystallography) meeting in Seattle, Washington. This esteemed crystallography conference which boasted the participation of no less than eight Nobel Prize winners took place in the magnificent Washington Convention Centre over a period of nine days, the last four of which were attended. Arriving on the "rest day" I dutifully relinquished the Panoramic

Tour of Seattle to give a seminar at the Centre of Bioengineering (University of Washington) where I was most warmly hosted by Gerry Pollack. The fibre diffraction session comprised three sub-sessions including 27 papers covering synthetic polymers (chaired by Kenn Gardner), methods of structure determination (chaired by John Blackwell) and fibre diffraction of biological polymers (chaired by Rick Millane). Reports and abstracts from these sessions are all available on the IUCr WWW page (<http://www.hwi.buffalo.edu/aca/>).